OOKAMI PROJECT APPLICATION

Date: **March 30. 2022**

Project Title: B-Spline R-Matrix and R-Matrix with Time Dependence Calculations for Electron and Photon Collisions

Usage:

☒ Testbed

☐ Production

Principal Investigator: Klaus Bartschat

University/Company/Institute:	Drake University / Physics & Astronomy
Mailing address including country:	2804 Forest Avenue Des Moines, IA 50311 USA
Phone number:	+1-515-954-9880
Email:	klaus.bartschat@drake.edu
Names & Email of initial project users:	**Klaus Bartschat** **(klaus.bartschat@drake.edu)** **Kathryn Hamilton** **(kathryn.hamilton@drake.edu)**

Usage Description: We plan to check whether OOKAMI is suitable for our B-spline Atomic R-Matrix (BSR) [1] and R-matrix with Time Dependence (RMT) [2] codes. These packages (written in FORTRAN-90 with OpenMP/MPI parallelization; no GPUs yet, but we are looking into that) are used to model atomic structure and time-independent electron collision and photoionization processes (BSR), as well as time-dependent, short-pulse, intense laser interactions with atoms and molecules (RMT). They are currently running well in production mode on Frontera, Stampede2, Bridges-2, and Expanse, all of which have a different architecture than OOKAMI. Since OOKAMI will become an XSEDE resource later this year, we should find out whether to include it in our next resource request.

[1] O. Zatsarinny, *BSR: B-spline atomic R-matrix codes.*
Comp. Phys. Commun. **174** (2006) 273
This is the only published version, but a lot has been some since.

[2] Andrew C. Brown, …, Kathryn R. Hamilton, et al., *RMT: R-matrix with time-dependence. Solving the semi-relativistic, time-dependent Schrödinger equation for general, multielectron atoms and molecules in intense, ultrashort, arbitrarily polarized laser pulses*.
Comp. Phys. Commun. **250** (2020) 107062

Computational Resources:

Total node hours per year: 15,000

Size (nodes) and duration (hours) for a typical batch job: 50 nodes / 10 hours
[We'll start much smaller, but if things work, these would be typical sizes for real tests.]

Disk space (home, project, scratch): 10 GB, 500 GB, 1 TB

Personnel Resources (assistance in porting/tuning, or training for your users**):**
Not known yet

Required software: BLAS, LAPACK, SCALAPACK (MKL preferred), cmake, Python

If your research is supported by US federal agencies:

Agency: National Science Foundation

Grant number(s): PHY-1803844, OAC-1834740, PHY-2110023. XSEDE-PHY-090031

Production projects:

Production projects should provide an additional 1-2 pages of documentation about how
(a) the code has been tuned to perform well on A64FX (ideally including benchmark data comparing performance with other architectures such as x86 or GPUs)
(b) it can make effective use of the key A64FX architectural features (notably SVE, the high-bandwidth memory, and NUMA characteristics)
(c) it can accomplish the scientific objectives within the available 32 Gbyte memory per node

N/A (Testbed project)